

## Web Tool for constructing a covariance matrix from EXFOR uncertainties

V.Zerkin, IAEA-NDS, 20/06/2011

Last few years there is growing interest and usage of covariances in nuclear data community. Covariance data in evaluated data files are used already very long time, have well defined formats (ENDF-6) and developed software of different types. Although EXFOR does not even have established formats for storage of covariance data, most of experimentalists could not provide these data – they published partial uncertainties which finally have appeared in EXFOR, and for some old experiments this information is absent at all. But even in the cases when information about uncertainties is very poor or absent, nowadays evaluators would like to be able to have some covariance matrix using some assumptions. Presented Web tool was developed for such evaluators, and also for experimentalists and EXFOR compilers who are interested in this subject. The tool was created in October-2010 and until now has status “under development”. The general ideas of algorithms are based on the relevant part of the methodology used in the work under IAEA Coordinated Research Project "Neutron Cross-section Standards" [1].

How it works.

1. The tool starts from converting EXFOR file to computational format C5 (C4 + systematic and statistical uncertainties) and presenting to user report with full relevant information:
  - C5 data points (energy, central values of cross sections)
  - C5 uncertainties (total, systematic, statistical)
  - all uncertainties given in EXFOR file
  - text from EXFOR given in ERR-ANALYS and METHOD sections
2. Then user can setup new values of uncertainties (or confirm existing uncertainties), introduce new (artificial) uncertainties splitting systematic uncertainties to parts, etc. This group will be used on the next step as input variables.
3. After that user defines how to use existing and newly introduced uncertainties for constructing covariance matrix: correlation type (uncorrelated, fully correlated and partially correlated). For partially correlated uncertainties (named medium energy range (MERC) correlation components in [1]) user defines additional parameters: correlation length and scale.
4. Finally user submits calculation and receives intermediate and final results in the following forms: raw data, data in ENDF-6 format (MF33) and link to Web-ZVView plotting package, where user can generate output in EXFOR format (draft) and text input for Fortran users including Fortran code.

The tool is available in the IAEA-NDS EXFOR Web retrieval system: <http://www-nds.iaea.org/exfor>; link [\[cov\]](#) will be offered to user for every dataset having Web-Quantity='CS'. EXFOR compilers can also use it when using EXFOR uploading system.

## **Concluding remarks**

Hopefully this tool can be practically useful for some users and may help in the development of the methods using experimental data with covariances for various applications. It will probably need further improvements and development. Suggestions and feed back are very welcome. It may also help in development of EXFOR formats for storage of the partial uncertainties.

## **Acknowledgment**

I thank to V.Pronyaev for useful discussions.

## **References**

1. V.G. Pronyaev, S.A. Badikov, A.D. Carlson, Chen Zhenpeng, E.V. Gai, G.M. Hale, F.-J. Hambach, H.M. Hofmann, T. Kawano, N.M. Larson, D.L. Smith, Soo-Youl Oh, S. Tagesen, H. Vonach, chapter “Evaluation Methodology and Codes”, pp.10-12, “International Evaluation of Neutron Cross-Section Standards”, IAEA-2006, [http://www-pub.iaea.org/MTCD/publications/PDF/Pub1291\\_web.pdf](http://www-pub.iaea.org/MTCD/publications/PDF/Pub1291_web.pdf)

## On-line help

**X4/Servlet: Help Title - Mozilla Firefox**

http://161.5.149.112/exfor1/x4js/x4covar\_hlp.htm

**Constructing covariance matrix from EXFOR uncertainties**

programmer: V.Zerkin (IAEA), consultant: V.Pronyaev (IPPE, Obninsk)  
International Atomic Energy Agency, October 2010  
(Status: under development)

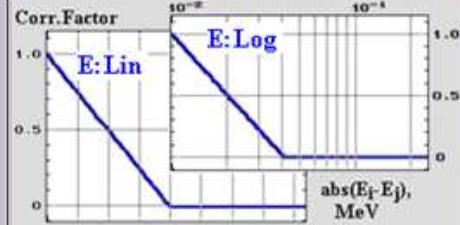
**MERC (Medium Energy Range Correlations).**  
*Applicable for partially-correlated uncertainties.*  
 The correlation length of partially correlated uncertainties (Medium Energy Range Correlation) is determined as energy range of which correlations between uncertainties in two energy points disappear\*. Log scale for energy correlations is probably more common for the time of flight measurements and linear scale - for discrete energy source measurements.

Typical examples of usage:

1) Scale:Lin; Energy: from 0 to 20MeV; Length: 0.1 (to 0.25)  
*(means: points farer than 2 MeV (20MeV\*0.1) are not correlated; between 0 and 2MeV, correlation factor = 1-abs( $E_i-E_j$ )/2MeV )*

2) Scale:Log; Energy: from  $10^{-5}$ eV to 20MeV; Length: 0.05  
*(means: points farer than 1/20 of the energy range are not correlated, otherwise correlation factor decreases from 1 to 0 proportionally to differences of energies in the logarithmic scale)*

3) User can choose Energy range corresponding to Min-Max of selected dataset, set up type of Energy scale to Lin/Log, and define correlation Length on the basis of own considerations



\*Note. This Web-tools presents an independent implementation of the algorithms of construction of covariance matrix for experimental data used under IAEA Coordinated Research Project "Neutron Cross-section Standards", 2004-2006 (see [\[page\]](#)).

**SERC (Short Energy Range Correlations).**  
*Applicable for uncorrelated uncertainties.*  
 Example: statistical uncertainties.

**LERC (Long Energy Range Correlations).**  
*Applicable for fully-correlated uncertainties*  
 Example: uncertainties in the determination of mass of the sample.

Uncorrelated SERC (Short Energy Range)	Fully-correlated LERC (Long Energy Range)	Partially-correlated MERC (Medium Energy Range)
1 0 0 0 0 0 0 0	1 1 1 1 1 1 1 1	1 .7 .4 -.1 0 0 0 0
0 1 0 0 0 0 0 0	1 1 1 1 1 1 1 1	.7 1 .7 .4 -.1 0 0 0
0 0 1 0 0 0 0 0	1 1 1 1 1 1 1 1	.4 .7 1 .7 .4 .1 0 0
0 0 0 1 0 0 0 0	1 1 1 1 1 1 1 1	.1 .4 .7 1 .7 .4 -.1 0
0 0 0 0 1 0 0 0	1 1 1 1 1 1 1 1	0 .1 .4 .7 1 .7 .4 .1
0 0 0 0 0 1 0 0	1 1 1 1 1 1 1 1	0 0 .1 .4 .7 1 .7 .4
0 0 0 0 0 0 1 0	1 1 1 1 1 1 1 1	0 0 0 .1 .4 .7 1 .7
0 0 0 0 0 0 0 1	1 1 1 1 1 1 1 1	0 0 0 0 .1 .4 .7 1

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Last modified: 11/04/2010 18:39:13  
 Project: EXFOR-Relational V.Zerkin, IAEA, 1999-2010

# Working Screenshot-1

Attachment-2.

**X4Covar - Mozilla Firefox**

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http://161.5.149.112/exfor1/servlet/X4sShowX4err?File=db&db=x4&op=

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X4Covar wp2011-32.pdf (application/pdf...) STANDARDS Data development...

**Constructing a covariance matrix from EXFOR uncertainties**  
by V.Zerkin (IAEA), consultant: V.Pronyaev (IPPE, Obninsk)  
International Atomic Energy Agency, October 2010

Request: #2590 File: X4R2590\_tdat.x4  
Dataset: 41487011 LX=166  
Reaction: 94-PU-240(N,F),,SIG  
C4Referer: A.B.Laptev,ET.AL. (07)

**Data and uncertainties (data points: 166)**

No.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	...
Energy (eV) *0.001	577.2	587.4	597.9	608.7	619.9	631.3	643.6	655.1	667.5	680.2	693.3	706.9	720.8	735.1	749.8	765.	780.7	796.9	813.5	830.7	84
Data (B) *1000.	548.	615.	750.	679.	717.	770.	811.	707.	884.	941.	866.	855.	1052.	955.	1085.	1089.	1046.	1047.	1161.	1213.11	

**Uncertainties defined in C4**

Total (%)	12.0	8.4	7.4	7.6	7.4	7.3	7.2	7.6	6.5	6.2	6.3	6.3	6.3	6.1	5.6	5.8	5.8	5.7	5.8	5.3	E
Statistical (%)	11.7	8.0	6.8	7.1	6.8	6.8	6.7	7.1	5.9	5.5	5.7	5.6	5.6	5.4	4.9	5.1	5.1	5.0	5.1	4.5	4
Systematic (%) empty	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	

**Uncertainties given in EXFOR**

ERR-S (%)	11.7	8.0	6.8	7.1	6.8	6.8	6.7	7.1	5.9	5.5	5.7	5.6	5.6	5.4	4.9	5.1	5.1	5.0	5.1	4.5	A
ERR-1 (%)	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	C
ERR-2 (%)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	D
ERR-3 (%)	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1
ERR-4 (%)	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2
ERR-5 (%)	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1
ERR-7 (%) const	0.1	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	
ERR-8 (%)	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	O

**Summary: available uncertainties L=11**  
**Text in EXFOR under keywords "ERR-ANALYS" and "METHOD"**

```
#ENTRY 41487 L=6
METHOD (TOF) 48.5 m flight path
Data-acquisitions system based on 100 MHz FLASH-ADC.
512 TOF channels x 128 pulse height channels array
was accumulated for each target nucleus.
(PHD) TOF and pulse-height spectra were accumulated as
two-dimensional matrix.

#/ENTRY 41487
#SUBENT 41487011 L=14
ERR-ANALYS (ERR-S) Statistical uncertainty (1 sigma)
Estimated systematic uncertainty caused by
(ERR-1)- separation of fission and background events in
pulse height spectra,
(ERR-2)- energy-independent neutron background,
(ERR-3)- energy-dependent neutron background.
```

**...Method Time-Of-Flight: Yes**  
**Set/Reset Values of C4-Uncertainties (%)**

Name	Status	Set all values to	Set if empty	Comment
Total	full	% of [Data]		[myErr-*] are uncertainties defined by user; they can be used e.g. to split [Systematic] uncertainty to components:
Statistical	full	% of Total		a) fully correlated and
Systematic	empty	Auto		b) medium energy range correlated
myErr-1	empty	75 % of Systematic		or for using uncertainties given in free EXFOR text under [ERR-ANALYS]
myErr-2	empty	25 % of Systematic		
myErr-3	empty	2 % of Data		

**Request Submit Reset  Submit in new Window**

Input Parameters for Calculation

Grouping Factor: 2 data points (required if final covariance matrix is too large)

No.	Name	Apply	Correlation-type	Parameters
1	Statistical	<input checked="" type="checkbox"/>	Uncorrelated	
2	Systematic	<input checked="" type="checkbox"/>	Fully-correlated	
3	myErr-1	<input type="checkbox"/>	Fully-correlated	
4	myErr-2	<input type="checkbox"/>	Partially-correlated	Corr-Length: 0.05 of the Range(eV): 1e-5 to 20e6 Scale: Log >>
5	myErr-3	<input type="checkbox"/>	Partially-correlated	Corr-Length: 0.05 of the Range(eV): 1e-5 to 20e6 Scale: Log >>

Page generated: 2011/05/21,17:15:21 by X4-Servlet on 161.5.149.112  
Project: "Multi-platform EXFOR-CINDA-ENDF", V.Zerkin, IAEA-NDS, 1999-2011  
Request from: vg-proxy2.iaea.org (161.5.131.43)

Find:     Match case  Reached end of page, continued from to

## Working Screenshot-2

Attachment-3.

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http://161.5.149.112/exfor1/servlet/X4sShowX4err

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X4Covar X4Covar wp2011-32.pdf (appl... STANDARDS Data de...)

**Covariance matrix from EXFOR uncertainties**  
by V.Zerkin (IAEA), consultant: V.Pronyaev (IPPE, Obninsk)  
International Atomic Energy Agency, October 2010

Request: #2590 File: X4R2590\_tdat.x4  
Dataset: 41487011 LX=83  
Reaction: 94-PU-240(N,F),,SIG  
C4Referer: A.B.Laptev,ET.AL. (07)

**Data**

No.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
Energy (eV) *0.001	582.3	603.3	625.6	649.05	673.85	700.1	727.95	757.4	788.8	822.1	857.65	895.5	935.95	979.15	1025.5	1075.	1128.5
Data (B) *1000.	581.5	714.5	743.5	759.	912.5	860.5	1003.5	1087.	1046.5	1187.	1268.	1326.	1377.	1495.5	1509.5	1570.5	1555.

**Uncertainties defined in C4**

Total (%)	7.6	5.6	5.6	5.6	4.9	4.9	4.8	4.5	4.5	4.4	4.1	3.8	3.8	3.7	3.7	3.5	3.6
Statistical (%)	7.1	4.9	4.8	4.9	4.0	4.0	3.9	3.5	3.5	3.4	3.1	2.6	2.5	2.5	2.4	2.1	2.2
Systematic (%)	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8

**Uncertainties given in EXFOR**

ERR-S (%)	7.1	4.9	4.8	4.9	4.0	4.0	3.9	3.5	3.5	3.4	3.1	2.6	2.5	2.5	2.4	2.1	2.2
ERR-1 (%)	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
ERR-2 (%)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ERR-3 (%)	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
ERR-4 (%)	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2
ERR-5 (%)	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2
ERR-7 (%) const	0.1	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=
ERR-8 (%)	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7

**Uncertainties set by user**

myErr-1 (%)	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4
myErr-2 (%)	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4
myErr-3 (%) const	2.0	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=

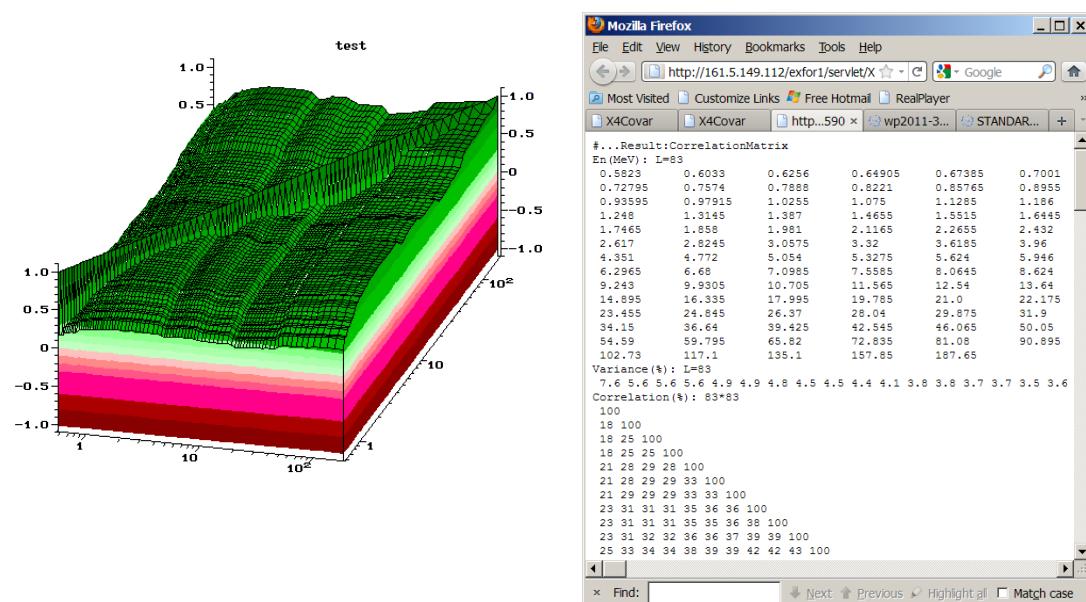
**Summary:** available uncertainties L=14  
**Text in EXFOR under keywords "ERR-ANALYS" and "METHOD"**  
 ...Method Time-Of-Flight: **Yes**  
**Calculations...**

**Final results:** [ENDF-MF33] [Plot] [Raw]

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 Project: "Multi-platform EXFOR-CINDA-ENDF", V.Zerkin, IAEA-NDS, 1999-2011

Find: Next Previous Highlight all Match case

## Plot and output data



## Working Screenshot-3

Example of intermediate output for controlling  
correctness of calculations

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http://161.5.149.112/exfor1/servlet/X4sShowX4err

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Index of /... X4Covar X4Covar wp2011... STANDAR... NRDC 2011 IAEA Nu... +

Dataset: 309980031 LX=19  
 Reaction: (69-TM-169(N,G)69-TM-170,,SIG)/(79-AU-197(N,G)79-AU-198,,SIG)  
 C4Referer: Xia Yijun,ET.AL. (88)

- Data and uncertainties (data points: 19)

No.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
Energy (eV) *0.001	11.2	12.9	14.	15.1	16.4	17.9	19.6	21.6	23.9	26.5	29.6	33.3	37.8	43.2	49.8	58.1	68.8	82.3	100.
Data (NO-DIM) *1.	2.26	2.13	1.82	1.91	1.82	1.66	1.65	1.82	1.8	1.69	1.71	1.77	1.79	1.72	1.83	1.76	1.65	1.71	1.72

**Uncertainties defined in C4**

Total (%) const	20.0	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=
Statistical (%) const	17.3	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=
Systematic (%) const	10.0	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=

**Uncertainties set by user**

myErr-1 (%) const	8.7	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=
myErr-2 (%) const	5.0	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=
myErr-3 (%) const	2.0	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=	=

+ Summary: available uncertainties L=6  
 + Text in EXFOR under keywords "ERR-ANALYS" and "METHOD"  
 ...Method Time-Of-Flight: Yes  
 - Calculations...

- 1)...add1matrix: name=Statistical type=[Uncorrelated] chk=[on] include=Yes  
 #SERC (Short Energy Range Correlation):  $a_{ii}=1$ ;  $a_{ij}=0(i \neq j)$
- 2)...add1matrix: name=Systematic type=[Fully-correlated] chk=[] include=No
- 3)...add1matrix: name=myErr-1 type=[Fully-correlated] chk=[on] include=Yes  
 #LERC (Long Energy Range Correlation):  $a_{ij}=1$
- 4)...add1matrix: name=myErr-2 type=[Partially-correlated] chk=[on] include=Yes  
 #MERC: Medium Energy Range Correlation

```
#MERC (Medium Energy Range Correlation) Matrix: a_ij
#Parameters: Lin/Log: 1; Energy: 1.000e-05 to 2.000e+07; Lenth: 0.05;
#####
  1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19
1) 11200   1
2) 12900   .90  1
3) 14000   .84  .94  1
4) 15100   .79  .89  .95  1
5) 16400   .73  .83  .89  .94  1
6) 17900   .67  .77  .83  .88  .94  1
7) 19600   .60  .70  .76  .82  .87  .94  1
8) 21600   .54  .64  .69  .75  .81  .87  .93  1
9) 23900   .46  .56  .62  .68  .73  .80  .86  .93  1
10) 26500   .39  .49  .55  .60  .66  .72  .79  .86  .93  1
11) 29600   .31  .41  .47  .52  .58  .64  .71  .78  .85  .92  1
12) 33300   .23  .33  .39  .44  .50  .56  .63  .69  .77  .84  .92  1
13) 37800   .14  .24  .30  .35  .41  .47  .54  .60  .68  .75  .83  .91  1
14) 43200   .05  .15  .20  .26  .32  .38  .44  .51  .58  .65  .73  .82  .91  1
15) 49800   0  .05  .10  .16  .22  .28  .34  .41  .48  .55  .63  .72  .81  .90  1
16) 58100   0  0  0  .05  .11  .17  .23  .30  .37  .45  .52  .61  .70  .79  .89  1
17) 68800   0  0  0  0  .05  .11  .18  .25  .33  .40  .49  .58  .67  .77  .88  1
18) 82300   0  0  0  0  0  0  .06  .13  .20  .28  .36  .45  .54  .65  .75  .87  1
19) 100000  0  0  0  0  0  0  0  0  .06  .14  .22  .31  .41  .51  .62  .74  .86  1
#####
  1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19
#/MERC-Matrix
5)...add1matrix: name=myErr-3 type=[Partially-correlated] chk=[] include=No
#/Calculations
```

Final results: [ENDF-MF33] [Plot] [Raw]